

The problem of quantum chaotic scattering with direct processes reduced to the one without

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Abstract

We show that the study of the statistical properties of the scattering matrix S for quantum chaotic scattering in the presence of direct processes (characterized by $\overline{S} \neq 0$, \overline{S} being the average S matrix) can be reduced to the simpler case where direct processes are absent ($\overline{S} = 0$). Our result is verified with a numerical simulation of the two-energy autocorrelation for two-dimensional S matrices. It is also used to extend Wigner's time delay distribution for one-dimensional S matrices, recently found for $\overline{S} = 0$, to the case $\overline{S} \neq 0$; this extension is verified numerically. As a consequence of our result, future calculations can be restricted to the simpler case of no direct processes.

The problem of chaotic wave scattering is of great interest in nuclear, molecular and mesoscopic physics, in optics and in the microwave domain. Common features have been found for system sizes spanning such a large range because of the generality of the phenomena involved.

In quantum-mechanical scattering problems with a chaotic classical dynamics one aims at studying the statistical properties of the scattering matrix S . Recently, this study has been further motivated by experiments on quantum electronic transport in mesoscopic systems [1].

The *one-energy* statistical distribution of the S matrix has been described successfully by an *information-theoretic* model that incorporates precisely the *physical information* that is relevant for a wide class of systems [2, 3, 4]. That information specifies: **1)** General properties: *i)* *flux*

conservation (giving rise to unitarity of the S matrix), *ii*) *causality* and the related analytical properties of $S(E)$ in the complex-energy plane, and *iii*) the presence or absence of time-reversal and spin-rotation symmetry, that determines the *universality class*: orthogonal, unitary or symplectic (designated as $\beta = 1, 2, 4$) [5, 6] and restricts further the structure of S : unitary symmetric, unitary or unitary self-dual, respectively. **2)** A specific property: the ensemble average $\langle S \rangle$, identified with the energy average \overline{S} , also known as the *optical S matrix* [7], which controls the presence of *prompt*, or *direct processes* in the scattering problem. In this procedure one constructs the statistical distribution of S using only the above physical information – expressible entirely in terms of S itself – without ever invoking any statistical assumption for the underlying Hamiltonian, that never enters the analysis. The resulting S -matrix distribution, known as *Poisson's kernel*, reproduces well the statistical scattering properties of ballistic cavities with a chaotic classical dynamics [4].

The joint statistical distribution of the S matrix at *two or more energies* has escaped, so far, an analysis within the philosophy described above (some aspects of the two-point problem have been studied assuming an underlying Hamiltonian described by a Gaussian ensemble, as in Refs. [8, 9]). An approach coming close to that philosophy was initiated in Ref. [10], with a study of the simplest quantity of a two-point character: the statistical distribution of the time delay –that involves the energy derivative of the S matrix– arising in the scattering process [11]. The physical motivation of Ref. [10] was the study of the electrochemical capacitance of a mesoscopic system [12]. The analysis was done for a cavity attached to one lead that can support only one open channel (so that $S = e^{i\theta}$ is a 1×1 matrix), for arbitrary β and $\overline{S} = 0$. It was based on a conjecture by Wigner [13], that assumes invariance of the statistics of the poles and residues of the related K matrix under the same transformation $S \rightarrow e^{i\phi/2} S e^{i\phi/2}$ that defines the invariant one-point measure [14] which, in the one-channel case, is $d\theta/2\pi$. That study was generalized to an arbitrary number of channels N in Refs. [15, 16], again for $\overline{S} = 0$: Wigner's conjecture was formulated and proved as the invariance of the k -point probability distribution of the N -channel S matrix under the transformation that defines the invariant measure for the universality class β .

Of physical importance is the case $\overline{S} \neq 0$: it corresponds to situations where direct processes are not negligible. For example, the case $\overline{S} = 0$ describes chaotic cavities with ballistic point contacts, while the coupling to leads containing tunnel barriers produces direct reflection and thus $\overline{S} \neq 0$

[4, 17]. A more complex combination of direct processes is described in Ref. [4].

In the present article we find a transformation that relates the k -point distribution of the N -channel S matrix for the case $\bar{S} \neq 0$ to that for $\bar{S} = 0$, thus relating the problems in the presence and in the absence of direct processes. In Ref. [18], the problem with a nondiagonal \bar{S} was reduced to that with a diagonal and real \bar{S} . Here we show that the problem can be reduced further to one characterized by $\bar{S} = 0$. That transformation, used in the past in relation with one-point functions [19], contains only the S matrix and its average \bar{S} . It is used here to extend to the case $\bar{S} \neq 0$ the time-delay distribution of Ref. [10] and is verified in this case by comparing our results with some known ones and with numerical simulations. It is also verified numerically for the two-point correlation function of two-dimensional S matrices. We believe that our result is appealing because of its conceptual simplicity and may open the way for further studies in this field.

We first summarize the information-theoretic model of Refs. [2, 3, 4]. The starting point is the measure $d\mu^{(\beta)}(S)$ for $n \times n$ S matrices, that remains *invariant* under the symmetry operation for the universality class β [5, 6, 14]. The ensemble average of S vanishes for the invariant measure, and so does the prompt component. An ensemble for which $\langle S \rangle = \bar{S} \neq 0$ contains more information than the invariant-measure: it can be constructed as $p_{\bar{S}}^{(\beta)}(S)d\mu^{(\beta)}(S)$ and the information associated with it is defined as $\int p_{\bar{S}}^{(\beta)}(S) \ln [p_{\bar{S}}^{(\beta)}(S)] d\mu^{(\beta)}(S)$. We assume to be far from thresholds and recall that $S(E)$ is *analytic* in the upper half of the complex-energy plane (causality) [20]. The study of the statistical properties of S is simplified by idealizing $S(E)$, for real E , as a *stationary random function* satisfying the condition of *ergodicity*, which in turn implies the equivalence of energy and ensemble averages [21]. We thus have the *analyticity-ergodicity* requirements (AE), that imply $\langle S_{ab}^p S_{cd}^q \dots \rangle = \langle S_{ab} \rangle^p \langle S_{cd} \rangle^q \dots$, so that averages of products of S -matrix elements not involving complex conjugation can be written in terms of the matrix $\langle S \rangle = \bar{S}$. The one-energy probability density

$$p_{\bar{S}}^{(\beta)}(S) = V_{\beta}^{-1} \frac{[\det(I - \bar{S}\bar{S}^{\dagger})]^{(\beta n + 2 - \beta)/2}}{|\det(I - S\bar{S}^{\dagger})|^{\beta n + 2 - \beta}}, \quad (1)$$

where V_{β} is a normalization constant, is known as Poisson's kernel: it satisfies the AE requirements [2] and the associated information is less than or equal to that of any other probability density satisfying AE for the same \bar{S} [3]. In Eq. (1), the elements of S are assumed to be complex numbers for

$\beta = 1, 2$ and quaternions for $\beta = 4$; for the definition of the determinant of a quaternion matrix, see Ref. [5], p. 126 .

Now consider the transformation

$$S_0 = t_1'^{-1}(S - r_1)(1 - r_1^\dagger S)^{-1}t_1^\dagger, \quad (2)$$

where r_1, t_1, r_1', t_1' are the $n \times n$ blocks of the matrix

$$S_1 = \begin{bmatrix} r_1 & t_1' \\ t_1 & r_1' \end{bmatrix}, \quad (3)$$

which has the symmetry associated with the universality class β . One can prove the following statement [2, 16, 17, 19]: if the one-energy distribution of S is Poisson's measure (1) and we identify r_1 in the transformation (2) with \overline{S} , the one-energy distribution of S_0 is the invariant measure $d\mu^{(\beta)}(S_0)$. In other words, the transformation (2), with $r_1 = \overline{S}$, transforms the problem with direct processes to one without ($\overline{S}_0 = 0$), as far as the one-energy distribution goes.

Now suppose that *at every energy E* we subject $S(E)$ to the transformation (2), always with the same \overline{S} . We prove below the following statement: *the joint statistical properties of the transformed $S_0(E_1), S_0(E_2)$, etc. are precisely the ones associated with the problem without direct processes, characterized by $\overline{S}_0 = 0$.* In other words, the above transformation relates $S(E)$, understood as a *stationary random function of energy*, for a problem with direct processes to one without.

We prove the above statement for S unitary and symmetric ($\beta = 1$), the proof for the other symmetries being similar. Consider first the case of \overline{S} diagonal and real. S can be written in terms of the real amplitudes $\gamma_{\lambda a}$'s and the energy levels E_λ 's, as

$$S(E) = [1 + iK(E)][1 - iK(E)]^{-1}, \quad (4)$$

where the K matrix is given by

$$K_{ab}(E) = \sum_{\lambda} \frac{\gamma_{\lambda a} \gamma_{\lambda b}}{E_{\lambda} - E}. \quad (5)$$

The $\gamma_{\lambda a}$'s are uncorrelated Gaussian variables and the E_{λ} 's follow the statistics of the Gaussian Orthogonal Ensemble [5, 6], with average spacing Δ . $\overline{S}(E)$ is given by [18]

$$\overline{S(E)}_{ab} = (1 - y_{aa})(1 + y_{bb})^{-1} \delta_{ab}, \quad (6)$$

where $y_{aa} = \pi \langle \gamma_{\lambda a}^2 \rangle / \Delta$. Just as S and K are related by Eq. (4), the transformed S_0 , Eq. (2), can be written in terms of a matrix K_0 given by

$$K_0 = i(1 - S_0)(1 + S_0)^{-1}. \quad (7)$$

Substituting the transformation (2) into (7), with S given by (4), we finally find

$$(K_0)_{ab} = y_{aa}^{-1/2} K_{ab} y_{bb}^{-1/2}. \quad (8)$$

Thus, the $\gamma_{\lambda a}$'s are rescaled by a constant ($\gamma_{\lambda a} \rightarrow y_{aa}^{-1/2} \gamma_{\lambda a}$), which is the appropriate one to ensure $\overline{S_0(E)} = 0$. Therefore, under the transformation (2), the $\gamma_{\lambda a}$'s retain their Gaussian distribution, while the energy levels E_λ 's are unchanged. We conclude that the statistical properties of the transformed random function $S_0(E)$ are the same as those of a statistical $S(E)$ matrix without direct processes. This proves our statement for \overline{S} diagonal and real. The case of arbitrary \overline{S} can now be reduced to the above one using the results of Ref. [18].

As a first application of the above statement, we extend to $\overline{S} \neq 0$ the time-delay distribution found in Ref. [10] for one spatial channel, $\overline{S} = 0$ and arbitrary β . We consider Eq. (2) for $n = 1$, with $r_1 = \overline{S}$; omitting the unimportant phase factor t_1^*/t_1 , we have

$$S_0(S) = (S - \overline{S})(1 - \overline{S}^* S)^{-1}, \quad (9)$$

where S_0 and S can be written as $S_0 = \exp(i\theta_0)$, $S = \exp(i\theta)$.

We are interested in the time delay [11] $\theta' = d\theta/dE$; we express it in terms of θ_0 and $\theta'_0 = d\theta_0/dE$ as

$$\theta' = d\theta/dE = \left[1 - |\overline{S}|^2 \right] \left| 1 + \overline{S}^* e^{i\theta_0} \right|^{-2} d\theta_0/dE \equiv f(\theta_0) \theta'_0. \quad (10)$$

To find the distribution of θ' we need the joint distribution of θ_0 and θ'_0 , $p_0^{(\beta)}(\theta_0, \theta'_0)$, which, being the one for no direct processes, factorizes as [15, 16]

$$p_0^{(\beta)}(\theta_0, \theta'_0) = p_0^{(\beta)}(\theta'_0)/2\pi. \quad (11)$$

It is convenient to express Eqs. (10) and (11) in terms of the variables u , u_0 defined as

$$u = 2\pi/\theta' \Delta, \quad u_0 = 2\pi/\theta'_0 \Delta_0, \quad (12)$$

where Δ and Δ_0 denote the average level spacing for the problems described by S and S_0 , respectively. The above proof shows that $\Delta = \Delta_0$, since the energy levels E_λ are unchanged by the transformation (2). Thus, using (12) and $u_0 = 2\pi/\theta'_0\Delta$, Eq. (10) becomes

$$u = u_0/f(\theta_0). \quad (13)$$

The joint distribution of the statistically independent variables θ_0, u_0 [see Eq. (11)], needed to find the distribution of u , is given by

$$P_0^{(\beta)}(\theta_0, u_0) = P_0^{(\beta)}(u_0)/2\pi, \quad (14)$$

where $P_0^{(\beta)}(u_0)$ was obtained in Eqs. (16), (17) of Ref. [10] [and denoted there by $\hat{P}(u)$] as

$$P_0^{(\beta)}(u_0) = \frac{(\beta/2)^{\beta/2}}{\Gamma(\beta/2)} u_0^{\beta/2} e^{-(\beta/2)u_0}. \quad (15)$$

From (13), (14), (15) we write the distribution of u , $P_{\bar{S}}^{(\beta)}(u) = \langle \delta[u - u_0/f(\theta_0)] \rangle$, as

$$P_{\bar{S}}^{(\beta)}(u) = \frac{1}{2\pi} \int f(\theta_0) P_0^{(\beta)}(f(\theta_0)u) d\theta_0 = \frac{(\beta/2)^{\beta/2}}{2\pi\Gamma(\beta/2)} u^{\beta/2} \int_0^{2\pi} [f(\theta_0)]^{1+\beta/2} e^{-\frac{\beta}{2}uf(\theta_0)} d\theta_0. \quad (16)$$

For the dimensionless time delay $\tau = 1/u = \theta'\Delta/2\pi$ we finally find the probability density

$$w_{\bar{S}}^{(\beta)}(\tau) = \frac{\left(\frac{\beta}{2}\right)^{\beta/2}}{2\pi\Gamma\left(\frac{\beta}{2}\right)\tau^{2+\frac{\beta}{2}}} \int_0^{2\pi} [f(\theta_0)]^{1+\frac{\beta}{2}} e^{-\frac{\beta}{2\tau}f(\theta_0)} d\theta_0. \quad (17)$$

The calculation of $w_{\bar{S}}^{(\beta)}(\tau)$ for arbitrary \bar{S} and β is thus reduced to quadratures [$f(\theta_0)$ is known, Eq. (10)] and the result coincides with our previous one [10] for $\bar{S} = 0$.

Eq. (17) is compared in Fig. 1 (a) with a numerical simulation that generates an ensemble of S 's from resonances sampled from an unfolded Gaussian ensemble for $\beta = 1$, the coupling amplitudes to the channel being independent Gaussian variables whose variance ensures $\bar{S} = 1/2$. The agreement is very good. Such a comparison was also made for $\beta = 2, 4$, although it is not illustrated here. For $\beta = 2$, Ref. [9] gives $w_{\bar{S}}^{(\beta)}(\tau)$ in analytical form

in terms of Bessel functions: we could not prove analytically the equivalence with our result; however, numerically the two are indistinguishable.

As a further verification of our statement, consider the autocorrelation function $c_{\overline{S}}(E) = \langle S_{11}^*(0)S_{11}(E) \rangle_{\overline{S}} - \langle S_{11}^*(0) \rangle_{\overline{S}} \langle S_{11}(E) \rangle_{\overline{S}}$. The quantity $|c_{\overline{S}}(E)|^2$ was calculated by generating numerically ensembles of 2×2 S matrices, with $\overline{S} = 0$ and $(1/2)I$, I being the unit matrix. To the data for $\overline{S} = (1/2)I$ the transformation (2) was applied: the results shown in Fig. 1 (b) are seen to be consistent with $|c_{\overline{S}=0}(E)|^2$.

Summarizing, we have found a transformation that relates the S matrix $S(E)$, understood as a stationary random function of energy, for a problem with direct processes ($\overline{S} \neq 0$) to one without ($\overline{S} = 0$). An application was made to extend Wigner's time-delay distribution for one channel S -matrices, from $\overline{S} = 0$ to $\overline{S} \neq 0$. A number of numerical simulations was made as a verification of our transformation. Our result implies that future work on the statistical properties of the S matrix can be restricted to the simpler case $\overline{S} = 0$, and extended to the case $\overline{S} \neq 0$ —corresponding to more complex scattering systems with direct processes—using the procedure described in this paper.

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Figure 1: (a) The distribution of time delays for one channel and in the presence of direct processes ($\overline{S} = 1/2$), for $\beta = 1$. The crosses are proportional to the theoretical probability density of Eq. (17), that was integrated numerically. The points with the finite-sample error bar are the results of the numerical simulation described in the text. The agreement is excellent. (b) The square of the autocorrelation function of the S_{11} element of a two-channel S matrix for $\beta = 2$ as a function of the energy separation, obtained from a numerical simulation. The open circles and diamonds correspond to $\overline{S} = 0$ and $(1/2)I$, respectively. The squares are the result of applying the transformation (2) to the data for $\overline{S} = (1/2)I$: they are seen to be consistent with the correlation for $\overline{S} = 0$.

